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Variable-Mesh Method of Solving Differential Equations

A multistep predictor-corrector method for the numerical solution of ordinary differential equations has been developed. The difference equations employed are generalizations, for the case of variable mesh spacing, of previous formulas requiring fixed step size. In addition to retaining the high local accuracy and convergence properties of the earlier methods, the variable-mesh method was developed in a form conducive to the generation of effective criteria for the selection of subsequent step sizes in the step-by-step solution of differential equations. These criteria are based on considerations of truncation error, convergence of corrector iterations, and an extensive treatment of relative numerical stability. The algorithm is of importance in the solution of practical problems arising in engineering and quantitative scientific research.

The variable-mesh multistep method has been tested by applying it to several single differential equations and to several systems of differential equations. This testing has given a fairly thorough demonstration of the effectiveness and reliability of the algorithm. One system of substantial importance for which the variable mesh approach proved especially effective was the problem of heat transfer to a supercritical fluid with variable physical properties and fully developed turbulent flow in a smooth tube. Another system was a stochastic model of enzymatically controlled cooperative unwinding and template replication of biological macromolecules. Most of the test problems were selected because of their inherent potential, both in the behavior of the solutions and in the behavior of the partial derivatives of the right hand sides of the equations with respect to the dependent variables, for producing numerical difficulties. Some are particularly suited to a variable-mesh treatment while others can

be solved efficiently with constant-mesh increments. In the latter cases it is important to note that the accuracy obtained by the variable mesh method was about the same as that obtained using constant increments with the same number of steps. This result indicates that the variable-mesh procedures do not have a degrading effect when they are used unnecessarily. Each equation was solved on the IBM System 360 using single precision starting values and double precision arithmetic to advance the solution. Values of δ , the target relative truncation error, ranging from 10^{-6} to 10^{-1} were used for each equation. The accuracy obtained was roughly proportionate to the values of δ specified. It was noted that the step lengths were limited almost entirely by the truncation error for the smaller values of δ with the stability/convergence criterion becoming of increasing importance with increasing δ .

Some of the problems were used in comparing the new algorithm with other fourth order numerical methods which also permit some variability in the mesh increments. The other methods used were the standard fourth order Runge-Kutta method, the Nordsieck method, and the basic Adams-Basforth/Adams-Moulton method, allowing doubling and halving of the increments with the latter. The new method proved superior to the other methods for these problems.

Note:

Documentation for the innovation is available from:

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(continued overleaf)

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